



INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
SHORT ABSTRACT OF THESIS

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Self-assembly of Small Molecules and Peptides: Relevant Applications
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SHORT ABSTRACT

The thesis entitled, "Self-assembly of Small Molecules and Peptides: Relevant Applications", is divided into six main chapters along with the experimental section and future directions. The thesis mainly contains supramolecular self-assembly, conformation, and morphology of small important organic molecules and important di-/tri-peptides and their application. Chapter 1: Self-assembly of small peptides has significant contributions to biological, chemical, and material science. Several important functional formed by self-assembly process such as nanostructures, e.g., nanotubes, nanofibres, nanoribbons, nanospheres, nanotapes, and nanorods. Modified Yamaguchi reagent plays as an efficient condensation reagent in several essential reactions. In chapter 2: we have developed the new modified Yamaguchi Reagent, 1-(2,4,6-trichlorobenzoyloxy)benzotriazole (TCB-OBt), and explored its structural and supramolecular characteristics. it formed a well-organized, continuous block-shaped structure. Moreover, this reagent provided significant yield under mild reaction conditions in amidation reactions. In chapter 3, we have demonstrated the effectiveness of various N-terminal protecting groups such as Boc, Fmoc, *o*-NBs, and *p*-NBs of Ant-Aib dipeptides on self-assembly. Interestingly, we have observed the generation of diverse nanostructures formation depending on N-terminal protecting groups and displayed different supramolecular packing in the solid state. Moreover, formed nano-vesicles have drug encapsulation and releasing properties. In chapter 4, we have described the self-assembly diversity of enantiomeric and reverse sequences of Ant and Phg containing dipeptides. Interestingly, structural and morphological homogeneity and heterogeneity were observed for enantiomeric and reverse peptide sequences. In chapter 5, we have discussed the self-assembly, conformation, and morphology of four Trp-containing dipeptides and their corresponding Phe-bearing dipeptides sequences. Interestingly, the significant morphological transition from various rod-like fiber structures to spherical structures was observed just by replacing Phe with Trp. In chapter 6, we have described the supramolecular insights of hetero-chiral protected tripeptides VFF (A β ₁₈₋₂₀) in solid and solution states. Interestingly, we have noticed different kinds of morphology by varying chirality of amino acids. In solid-state, peptides formed various supramolecular architectures. Moreover, all tripeptides peptides have a ThT binding affinity.

The developed reagent can be further used in other organic transformations. We can further explore various important di-, tri-, or tetra- peptide-based supramolecular assembly in solution and solid-state and find their application.